MICROSCOPIC CALCULATION OF EXPANDING NUCLEAR MATTER

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Quantum Molecular Dynamics (QMD) calculations are used to study the expansion phase in central collisions between heavy nuclei. The final state of such a reaction can be understood as the result of a entropy conserving expansion starting from a compact source. The properties of this hypothetic source, however, are in conflict with the assumptions used in fireball models. Moreover, this hypothetical source is not formed in the dynamical evolution of the system.

1 Introduction

The question how matter behaves under extreme conditions has initiated a large number of theoretical and experimental investigations [1]. In particular central collisions between two heavy nuclei are known to lead to a configuration where the density exceeds that of ordinary nuclei and the momentum distribution does not correspond to that of a Fermi gas at zero temperature. One speaks about the creation of hot and dense nuclear matter. There is quite some evidence from hydrodynamical calculations [2] as well as from the quantum statistical analysis of the fragmenting source in central collisions [3] that the hot and dense systems expands and cools along isentropes in the temperature-density plane. Moreover, so called fireball models [4], which assume an (isentropic) expansion from an equilibrated source have been applied with some success to describe data.

On the other hand it is still an open question, to which extent the system equilibrates before expanding and hence allows for the application of thermodynamical concepts. In this contribution we address the question, to which extend the final state of a heavy ion reaction can be interpreted as the result of an isentropic expansion and which conclusions about the high density stage can be drawn from the knowledge of the final momentum distribution only.

First the basic features of the Quantum Molecular Dynamics model with Pauli-potential are briefly reported. The source of irreversibility in microscopic transport models is discussed with this particular example. A novel method of reverting an isentropic expansion is introduced. Implications on the appli-

cability of equilibrium models are critically examined.

2 Quantum Molecular Dynamics with Pauli-Potential

Quantum Molecular Dynamics (QMD) [5,6,7] is a semi-classical model which calculates the trajectory of a heavy ion collision in the entire many-body phase-space. It simulates the many-body dynamics due to the real and imaginary part of the optical potential by merging two transport theoretical approaches: The real part of the potential is treated via a phenomenological nucleon-nucleon interaction, whereas the effect of the imaginary part can be translated into a collision term of the Boltzmann type [8]. QMD therefore contains a classical molecular dynamics section and a collision term, which performs a Monte-Carlo integration of the local collision kernel in a similar manner as in intranuclear cascade models [9].

Special attention has been given to the fermionic character of the nucleons in the molecular dynamics part as well. For an antisymmetrized state of two gaussian wavepackets the expectation value of the kinetic energy operator reads

$$E_{\rm kin} = \frac{p^2}{2\mu} + \frac{3\alpha\hbar^2}{4\mu} + \frac{\alpha\hbar^2}{2\mu}\frac{\alpha r^2 + \frac{p^2}{\alpha(\hbar c)^2}}{\exp\left\{\alpha r^2 + \frac{p^2}{\alpha(\hbar c)^2}\right\} - 1}\,, \tag{1}$$

where the second term on the right hand side is due to the zero point energy of the wavepackets. Since the width parameter α is time-independent and the corresponding energy cannot be transformed into other forms of energy this constant term is neglected. The third term can be interpreted as a coordinate- and momentum-dependent potential between the two gaussians [10]. However, in our case we took another functional form of the Pauli-potential [11]

$$V_{\rm Pauli} = V_0^{\rm Pauli}\left(\frac{\hbar}{p_0 q_0}\right)^3 \exp\left\{-\frac{(\boldsymbol{x}_j - \boldsymbol{x}_k)^2}{2q_0^2} - \frac{(\boldsymbol{p}_j - \boldsymbol{p}_k)^2}{2p_0^2}\right\}\delta_{\tau_j\tau_k}\delta_{\sigma_j\sigma_k}\,, \tag{2}$$

whose parameters have been adjusted to the temperature- and density-dependence of the kinetic energies of a free Fermi-gas [7]. The delta-functions indicate that this potential acts only between particles with identical spin and isospin projection.

Taking into account Fermi momenta in such a manner allows for a self-consistent determination of nuclear ground-states by searching for that configuration, which binds $A - Z$ neutrons and Z protons and minimizes the total energy. Necessary conditions for this minimum are

$$\frac{\partial H^A}{\partial \boldsymbol{p}_j} = \dot{\boldsymbol{r}}_j = \boldsymbol{0} \quad \text{and} \quad \frac{\partial H^A}{\partial \boldsymbol{r}_j} = -\dot{\boldsymbol{p}}_j = \boldsymbol{0}\,, \qquad j = 1, \ldots, A\,. \tag{3}$$

From the last equation we can conclude that these model nuclei are absolutely stable, because none of nucleons moves nore there is force acting on any of the

constituents.

In the following, we refer to QMD with the collision term switched off as molecular dynamics (MD). However, one has to keep in mind that the nucleons in the model do not behave as classical particles. The usage of a momentum-dependent potential implies that velocity and momentum of the particles are not proportional to each other.

3 Time-Reversibility of Molecular Dynamics

In order to prove the reversibility of the molecular dynamics section in the QMD model, we performed a molecular dynamics calculation of the system Au + Au at an incident beam energy of 150 MeV/nucleon and an impact parameter of 3 fm. This is a typical heavy ion reaction, which has been studied experimentally with the Plastic-Ball more than a decade ago [12] and has received novel attention because of the more recent investigations with the FOPI-detector at GSI [13].

The system is propagated on its molecular dynamics trajectory for a typical collision time of 400 fm/c. Then the momenta of all particles are mirrored and the system is propagated back with a negative time-step for another 400 fm/c. Stages during the back-progation are labelled with a prime, e.g. the instant 160' fm/c corresponds to a propagation for 400 fm/c with a positive time step width and an backpropagation for additional 240 fm/c with a negative time step width. In case of perfect reversibility the particles' positions in configuration space at that instant should be identical with the situation after 160 fm/c. Fig. 1 shows typical snap shots of coordinate- and momentum-space projections during the molecular dynamics simulation. Starting from two initially well separated gold nuclei (bottom row, 0 fm/c), in the course of the reaction the system partially disintegrates into light fragments and a few very heavy clusters, although no hard scatterings are involved (middle row, 400 fm/c). This kind of fragmentation is exclusively caused by the internucleon potentials. After the back propagation is completed (top row, 0' fm/c) projectile and target have formed again, which illustrates the time reversibility of MD.

To be more quantitative, the spectrum of distances between the positions in the initial state and those after the full propagation there and back have been calculated. The mean displacement is less than 1 fm in configuration- and 50 MeV/c in momentum-space. This is mainly due to too a coarse discretization when the high densities are reached.

The results presented have been obtained with default model parameters, which are employed in the simulations too. Using higher order integration routines and/or smaller time-steps could improve the agreement even more.

However, in view of the fact that the dynamics at short relative distances will be governed by hard collisions, the results of QMD calculations are not affected by this discretisation error.

4 Reverting an Isentropic Expansion

The time-reversal symmetry of the MD calculations shows that system follows an isentropic path. It is tempting to use the concept of the back propagation in order to time-revert the expansion of a simulated heavy ion collision, which is assumed to conserve the entropy . A typical evolution of a single event is shown in Fig. 2. In contrast to Fig. 1 the Au + Au system is propagated on its QMD trajectories, including the hard scatterings. Hence entropy may be produced during the compression–decompression dynamics. Again, the calculation is carried out for 400 fm/c and the back-propagation is carried out using MD only.

With collisions included (QMD-MD), the time-evolution drastically differs from the MD-MD calculation. The system fragments more violently, the spectators bounce off the hot and dense participant matter and the typical flow ellipsoid develops in momentum space. In contrast to the MD-MD calculation shown in Fig. 1 the QMD-MD simulation nolonger leads back to two well separated nuclei. All particles seem to stem from a single compact source. In momentum-space, however, the nonisotropic emission pattern is present, even after the backpropagation is completed.

The future evolution of a classical dynamical system in general is strongly dependent on the distribution of matter in phase-space. In particular the initial correlation between configuration and momentum space determines the dynamics.

In order to study the physics of the expansion phase in more detail, we have calculated the time-evolution of the one-body distribution function in QMD. Technically this is achieved by superposition of many events with the same incident energy and impact parameter. The result of this procedure is equivalent to a testparticle distribution of a VUU/BUU calculation. It allows for determination of the local velocity distribution with arbitrary precision, which is only limited by the number of events. The first and the second moment of the local velocity dsitribution are related to collective motion and the local temperature respectively.

Fig. 3 compares the distribution of matter and the local collective motion in the event-plane after the isentropic backpropagation until the highest density is reached again (left) with the corresponding stages on the system's true dynamical path (right).

Although the backpropagated state also exhibits a central density of twice the saturation density, the correlation between space and momentum shows a behaviour which is never observed in the ordinary QMD simulation. It shows that the final state of a heavy ion reaction can indeed be understood as the result of an isentropic expansion from a single compact source. However, the correlation between configuration and momentum-space has never really been traversed by the system.

A further analysis of the backpropagated starting point of the isentropic expansion is displayed in in Fig. 4. The mean directed transverse momentum as a function of rapidity, which is observed in the final state of the reaction survives the isentropic backpropagation almost completely. Only the rapidity distribution widens a bit compared to the final state. Again it is recognized that the isentropic backpropagation preserves the collective flow correlations. These correlations are just starting to develop in the corresponding temporal stages during the QMD propagation to the final state, which are shown as lines in the figure.

5 Summary

In summary, we have shown that the transport mechanism in the QMD model can be divided into an entropy conserving part and a stochastic part which is the underlying microscopic cause of the newly produced entropy in heavy ion reactions. The time-reversal symmetry of the classical equations of motion allows for a reversion of the anticipated isentropic expansion in the simulation.

The hypothetical starting point of the isentropic expansion of nuclear matter in heavy ion collisions indicates that all matter stems from a single compressed source. On the other hand, the position–velocity correlations observed after the isentropic backpropagation differ drastically from those present in the corresponding reaction. The present analyses suggest that fireball models which assume an isentropic expansion from a compact source may describe data, if flow correlations were taken into account. However, the trajectories do not correspond to the true dynamical path of the system. This is due the fact that entropy is produced via abundant two body scatterings not only in the high density phase but also during the expansion.

Acknowledgments

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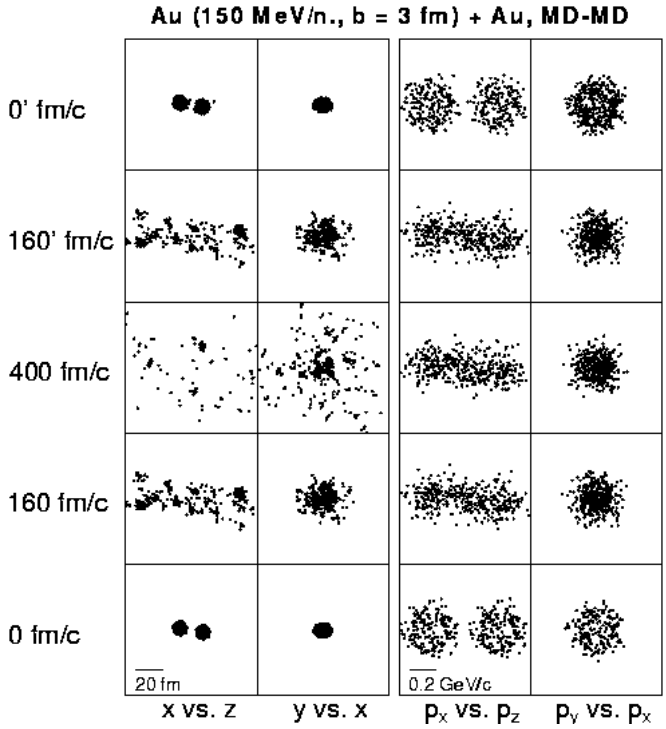

Figure 1: Position and momenta of nucleons in a classical molecular dynamics calculation of the reaction Au (150 MeV/nucleon, b = 3fm) + Au. After propagation for 400 fm/c, the momenta are mirrored and the system is propagated back for another 400 fm/c. Projections in configuration space (1st and 2nd column) and in momentum space (3rd and 4th column) onto the event plane (1st and 3rd column) and onto the plane perpendicular to the beam axis (2nd and 4th column) are displayed.

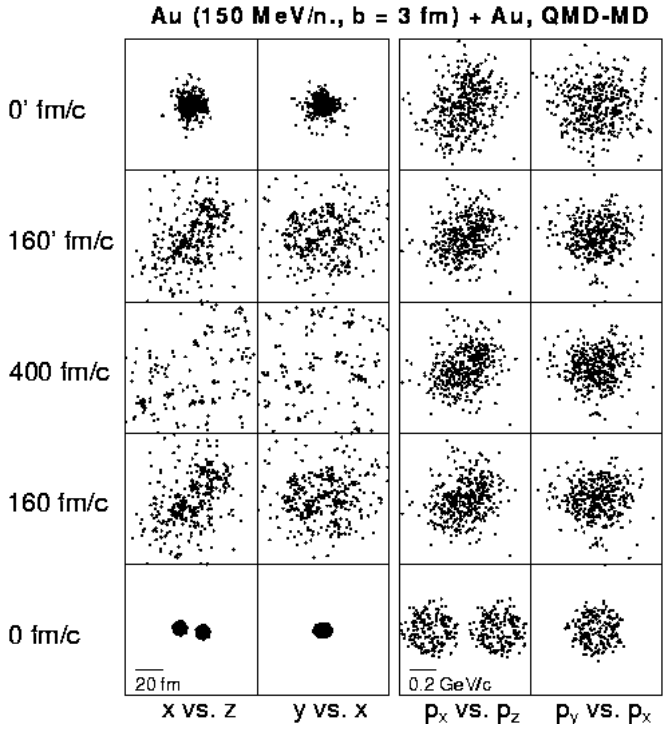

Figure 2: Same as Fig. 1 but for a MD back propagation after a full QMD propagation.

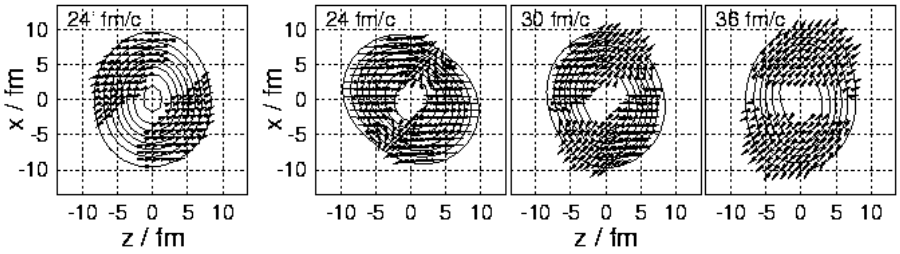

Figure 3: The backpropagated hypothetical starting point of an isentropic expansion (left) is compared to the corresponding reaction stages (right). The results have been obtained for Au (150 MeV/nucleon, b=3fm) + Au collisions, and show a cut through the reaction plane. The distance between two contour lines is $0.2\varrho_0$. The outermost contour indicates a density of $0.2\varrho_0$. The arrows indicate the collective motion. Only arrows corresponding to velocities larger than 0.05 c are displayed.

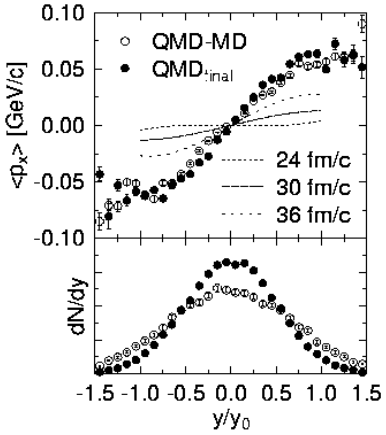

Figure 4: Flow correlations and rapidity distributions in the final state (closed circles) are compared to those of the state of maximum density in the backpropagation (open circles). The molecular dynamics trajectories preserve almost completely the flow correlations. Some of the $\langle p_x \rangle(y)$ curves during the QMD propagation are shown as lines.